

1,3-Dimethyl-4-ethylbenzene
874-41-9 | DTXSID0061246

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.11 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.21e-01

Confidence level: 8.51e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>2,3,5-Trichlorophenol</div> <div>Measured: 1.03</div> <div>Predicted: 1.61e-02</div>	<div>Image not found</div> <div>Monolinuron</div> <div>Measured: 9.39e-01</div> <div>Predicted: 1.71e-05</div>	<div>Image not found</div> <div>Cyclohexyl acetate</div> <div>Measured: 3.00</div> <div>Predicted: 2.43</div>
<div>Image not found</div> <div>1,3-Dimethyl-5-ethylbenzene</div> <div>Measured: 7.48e-01</div> <div>Predicted: 9.69e-01</div>		